TWO-PHASE FLOW MODELING WITH TOUGH2 OF A WASTE GEOLOGICAL REPOSITORY WITHIN THE FORGE PROJECT

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ABSTRACT

FORGE (Fate Of Repository Gases), a four-year (2009–2013) international research project supported by funding under the European Commission FP7 Euratom programme, is dedicated to the understanding of gas generation and migration as part of the quantitative assessment of a waste geological repository. Within the FORGE project, Work Package 1 is dedicated to the numerical modeling of a two-phase flow system (gas, mainly hydrogen as a result of corrosion and groundwater) in a radioactive waste geological repository. Several exercises were proposed that cover the modeling of a waste geological repository from the disposal cell scale to the repository scale with different codes. Special emphasis was placed (during the definition of the exercises) on the role of the EDZ and of the interfaces between materials, which could act as a conduit for preferential flow. During the calculations of the cell-scale benchmark, some convergence problems were encountered and will be described here. Some changes were made in the TOUGH2 code (Pruess, Oldenburg et al. 1999) to make implementing the prescribed conditions and parameters of the benchmark possible. The results of the calculations performed with different codes show that TOUGH2 obtains comparable results under the numerically challenging conditions defined in the exercise. This paper shows the results of the cell-scale benchmark obtained by ENSI with TOUGH2.

INTRODUCTION

Several benchmark exercises have been defined within the first work package of the FORGE project. The starting point for the definition of the exercises was a general agreement that the reference exercises will be as generic as possible and more aimed at studying how the system reacts rather than an intercomparison of codes. A second agreement was that the first exercise should be rather simple and at cell scale, aiming at a stepwise approach at a repository scale. The proposed calculation domain for the first exercise is shown in Figure 1 (Wendling, Yu et al. 2010).

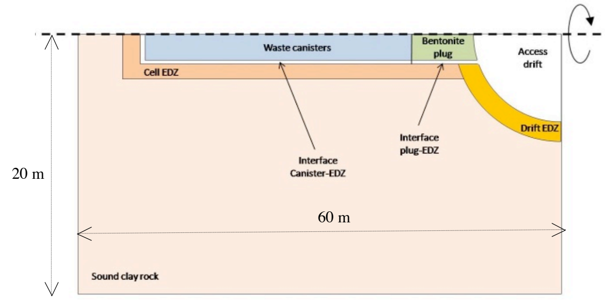

Figure 1. Domain of the model proposed for the first exercise.

The calculation domain is axisymmetric around the waste canister, with the effect of gravity in the vertical direction not considered. A gas production term provided for the disposal cell is imposed on an external surface of a cylinder representing the canister (blue domain in Figure 1). The canister material is considered impermeable to both water and gas, and therefore it is not explicitly represented in the model. The materials to be taken into account in the simulation include the EDZ of both the cell and the access drift, the cell plug, the backfill of the access drift, and the geological medium. The interfaces around the EDZ are considered in the model, with the material properties different for the interface facing the canister and for the interface facing the bentonite.

The objective of this benchmark is to better understand numerically the mechanisms of gas transport at the cell scale, and in particular to analyze the effect of the presence of different materials and interfaces on such mechanisms.

PARAMETERS: INITIAL AND BOUNDARY CONDITIONS

Important parameters prescribed for the benchmark at a reference temperature of 20°C are listed in Table 1 and Table 2.

Table 1 Material parameters for the interfaces and drift.

Parameter (at 20°C)	Materials		
	Interface facing plug	Interface facing canister	Backfill (access drift)
K_v [m^2]	5.0 10^{-18}	1.0 10^{-12}	5.0 10^{-17}
K_h [m^2]	1.0 10^{-17}	Kv=Kh	
Porosity [%]	30	100	40
Specific storage coefficient [m^{-1}]	4.6 10^{-06}	4.6 10^{-06}	1.0 10^{-05}
Two-phase flow parameters			
S_{gr} [%]	0	0	0
S_{wr} [%]	0	0	0
Van Genuchten parameters			
n [-]	4	4	1.5
P_r [Pa]	10^4	10^4	2 10^6
τ (Tortuosity)	1	1	2

One of the objectives of this benchmark is to study the effect of interfaces as preferential paths for the gas. For example, the interface facing the canister has a thickness of 1 cm and an intrinsic permeability of 10^{-12} m^2. The interface facing the bentonite has the same thickness and intrinsic permeability of 10^{-17} m^2.

The following expressions of the relative permeability for water and gas were proposed to be used in this benchmark:

$$k_r^w = \sqrt{S_{we}}\left[1-\left(1-S_{we}^{1/m}\right)^m\right]^2 \quad [1]$$

$$k_r^g = \sqrt{1-S_{we}}\left[1-S_{we}^{1/m}\right]^{2m} \quad [2]$$

Over the first 10,000 years, we imposed a constant production term for gaseous hydrogen of 0.2 kg/a as source term.

Table 2. Material parameters for bentonite, EDZ, and host rock.

Parameter (at 20°C)	Materials		
	Bentonite plug	EDZ	Geologial Medium
K_v [m^2]	1.0 10^{-20}	5.0 10^{-18}	5.0 10^{-21}
K_h [m^2]	Kv=Kh	1.0 10^{-17}	1.0 10^{-20}
Porosity [%]	35	15	15
Specific storage coefficient [m^{-1}]	4.4 10^{-06}	2.3 10^{-06}	2.3 10^{-06}
Two-phase flow parameters			
S_{gr} [%]	0	0	0
S_{wr} [%]	0	0	0
Van Genuchten parameters			
n [-]	1.6	1.5	1.5
P_r [Pa]	1.6 10^7	1.5 10^6	1.5 10^7
τ (Tortuosity)	4.5	2	2

The initial saturation of the rock and of the EDZ is 100%, and the initial water pressure is 5 MPa. Initial saturation for the interface is 5%, and for the drift and bentonite 70%. The gas pressure for partially saturated materials is 1 atm; water pressure is obtained according with van Genuchten models.

As indicated in Figure 2, time-dependent boundary conditions are prescribed on the drift for the water pressure and water saturation. The rest of the boundary conditions are shown in the next figure.

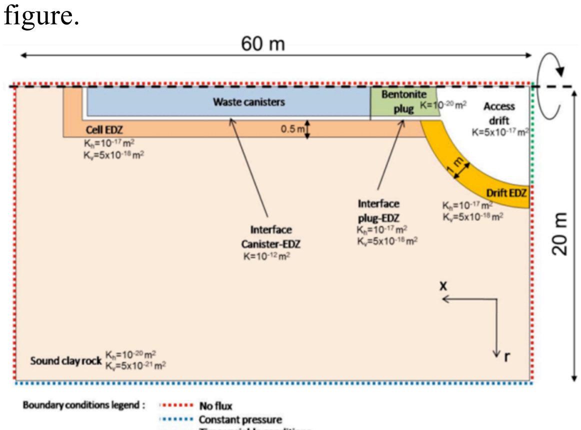

Figure 2. Representation of the model together with important parameters and boundary conditions.

IMPLEMENTATION OF THE MODEL WITH TOUGH2/TOUGH2-MP

To reduce the differences between the results of the different teams using the different codes, ENSI attempted to implement the parameters and models as prescribed in the exercise. Some of them, like the thin interfaces and the time-dependent boundary conditions, were difficult to implement in TOUGH2. The simulations were initially performed with TOUGH2 but some difficulties were found, such as the implementation of time-dependent boundary conditions and (above all) the long computational times. To reduce (as much as possible) these limitations, we decided to use the code TOUGH2-MP (Zhang, Wu et al. 2008), which is the parallel version of TOUGH2 developed also by Lawrence Berkeley National Laboratory. Our computer cluster consists of IBM AIX machines; this computer architecture was not included among the systems in which the program was tested. Therefore, the compiling options had to be adapted to our system, and additional features had to be installed in it. The code also requires the external libraries AZTEC and METIS. Compilation of these libraries was also system dependent, and besides, no compiling options were specified for our system.

After the installation of TOUGH2-MP, some tests were performed with inputs included in the distribution. The existing input for TOUGH2 was adapted to the code TOUGH2-MP, although in fact there are some slight differences between the input definitions of the two codes. After an extensive check of the code, we noticed that some lines had to be implemented in the code in order to be able to use TOUGH2-MP with our computer architecture.

Compared to the same simulations performed with TOUGH2, we observed that the code TOUGH2-MP ran faster at the beginning, but after some hundred years of simulation time, the codes start slowing down. In a first approach to the benchmark, the interface layer was modeled using three layers of nodes. Due to the small dimensions of the node elements in the interface, the code was very slow after some hundred years. It was therefore decided to use only one layer of nodes at the interface, which reduced the computation time.

The prescribed model for the gas relative permeability given by the van Genuchten-Mualem relation (γ=0.5) in Equation (2) is not available either in TOUGH2 or in TOUGH2-MP. The code was modified to allow this expression for the gas relative permeability; however, this option causes a slowdown of and instabilities within the code. Moreover, for a few calculations cases, we experienced a crash of the simulation after 10,000 years' time.

Some differences were also observed between the diffusion coefficients of hydrogen in the gas and liquid phase. Changes were made in the code TOUGH2/TOUGH2-MP to adapt it to the specifications. The diffusion coefficients of dissolved hydrogen in the binary hydrogen/water vapor mixture of the porous medium was specified in the benchmark as:

$$D^g_{H_2/vap} = (1 - S_w)\left(\frac{\phi}{\tau^2}\right) D_0 \left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)^{1.75} \qquad \textbf{[3]}$$

whereas in TOUGH2/TOUGH2-MP, the equivalent expression is given by:

$$D^g_{H_2/vap} = \phi \tau_0 \tau_\beta \left(\frac{1}{\tau^2}\right) D_0 \left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)^{1.75} \qquad \textbf{[4]}$$

Equivalently the expression for the diffusion coefficient of dissolved hydrogen in the waster of the porous medium is given by:

$$D^w_{H_2} = S_w \left(\frac{\phi}{\tau^2}\right) \times 1.57 10^{-14} \frac{T}{\mu_{water}(T)} \qquad \textbf{[5]}$$

In TOUGH2/TOUGH2-MP, the equivalent expression is given by:

$$D^w_{H_2} = \phi \tau_0 \tau_\beta \left(\frac{1}{\tau^2}\right) \times 1.57 10^{-14} \frac{T}{\mu_{water}(T)} \qquad \textbf{[6]}$$

Also, the expression for Henry's law proposed in the FORGE project is somewhat different from the one used in the TOUGH2/TOUGH2-MP code. Specifically, the expression proposed in FORGE contains the concentration of hydrogen in mol/m^3, whereas the expression in TOUGH2 uses the mol fraction of hydrogen. A conversion factor was implemented in the TOUGH2/TOUGH2-MP code to adapt it to the prescribed expression.

The influence of the initial conditions on the behavior of the system was studied with numerical simulations. We found that the numerical convergence of the simulations were improved if the initial conditions through the different nodes in the interface, EDZ and host rock changed smoothly. The best convergence was obtained when the initial conditions of the EDZ and the interface are the same. The results of ENSI and other teams confirm that, assuming the prescribed initial conditions, an initial transient of pressure occurs during the first thousandth of a year, as shown in Figure 3. This is explained by the different initial saturations of the interface (5%) and the EDZ (100%).

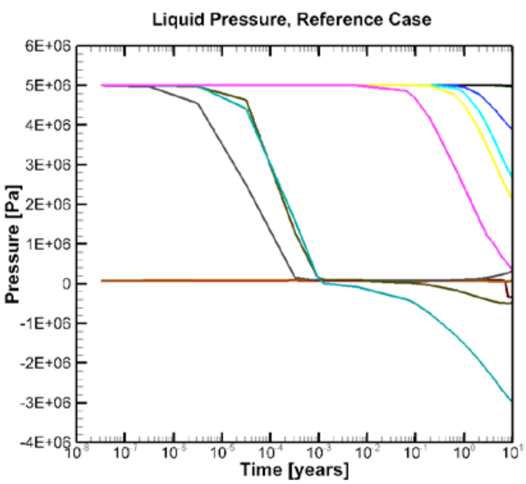

Figure 3. Values of the liquid pressure during the first ten years in different points of the model.

Initially, TOUGH2 was used to perform the simulations for this exercise. Also initially, the prescribed variations in pressure and saturation were implemented with a time-dependent source term. In this way, a variable mass of gas was introduced into the system, the effect of which required analysis. To avoid possible correlations with the inserted gas, another strategy was followed. The code TOUGH2-MP, unlike TOUGH2, includes the capability of implementing time-dependent boundary conditions for the pressure. As in the exercise, not only time-dependent boundary conditions for pressure but also for saturation were prescribed: the code had to be modified to allow the implementation of time-dependent saturation values as boundary conditions. The time-dependent boundary conditions caused the code to slow down, because it was realized after comparing calculations with and without time-dependent boundary conditions.

Since the model is axisymmetric around the axis of the cell, each element of the grid includes all elements generated by rotating each planar element around this axis. Therefore, intrinsic horizontal permeabilities are implemented in the input as prescribed, but intrinsic vertical permeabilities for the rotated elements can take values limited by the values of the horizontal and vertical permeabilities. Therefore an averaged value around the rotation axis was taken for the vertical intrinsic permeabilities.

The table below shows the calculation cases defined for this benchmark. Gas flux and dissolved hydrogen values through the defined surfaces are required, as well as values for water and gas pressure and saturation at different points and along the vertical and horizontal lines defined on the model. The considered points and an example of a vertical line are indicated in Figure 4.

Table 3. Calculation cases for the cell-scale benchmark

Reference Case	Parameter and conditions as specified before
Sensitivity analysis 1	EDZ intrinsic permeability equal to the one of the undisturbed rock (reduction of EDZ intrinsic permeability)
Sensitivity analysis 2	Power law for EDZ and host rock intrinsic permeability
Sensitivity analysis 3	Increase of diffusion coefficient of dissolved hydrogen
Sensitivity analysis 4a/4b	Delay of gas production of 1 year/ 2 years
Sensitivity analysis 5a/5b	Intrinsic permeability interface = 10^{-15} m^2/ Intrinsic permeability of the interface equal to the one of the EDZ
Sensitivity analysis 6	Mesh refinement

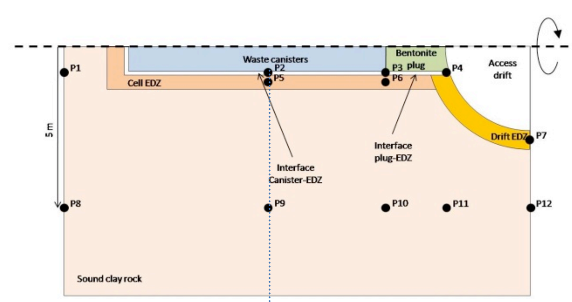

Figure 4. Schematic representation of the points as well as a vertical line where results are provided.

SOME RESULTS FOR THE REFERENCE CASE

In this section we present a selection of results for the reference case. The saturation close to the interface remains practically 100% until approximately 10,000 years, when it decreases but no less than 80%—as shown in Figure 5, which represents the variation of the saturation along a vertical line starting at the interface as shown in Figure 4.

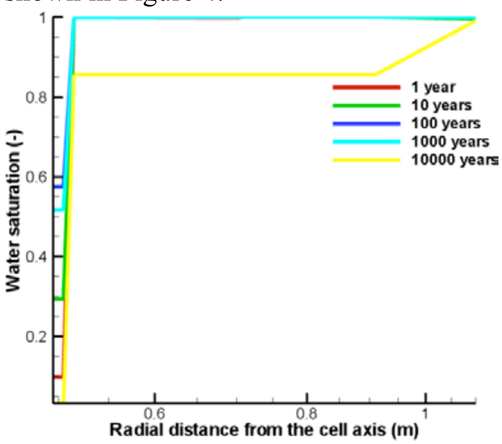

Figure 5. Variations in the saturation along a vertical line starting in the interface as shown in Figure 4.

The values of the saturation around the repository are shown in Figure 6. A detailed view of the interface facing the bentonite plug is also shown at the top.

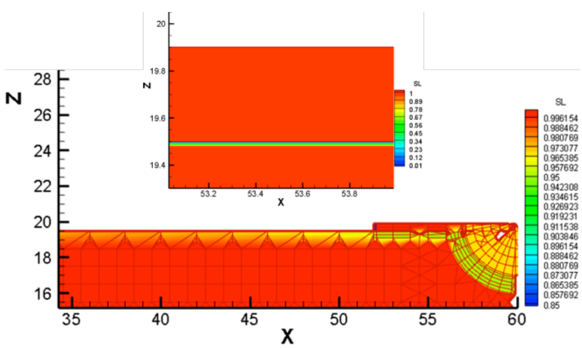

Figure 6. Results for the water saturation after 10000 years for the reference case. On the top a detail of the interface facing the bentonite plug is shown.

It can be observed in Figure 6 that, because of the very small permeability of the argillites and its high capillary entry pressure, desaturation occurs primarily inside the cell and up to the radial end of the EDZ, but the undisturbed argillites are not significantly desaturated. A tiny desaturation of the host rock close to the EDZ occurs. The interface is initially highly desaturated, but then partial resaturation occurs rapidly (10 years) before a general desaturation dominates the remaining years (Figure 5).

The evolution of gas pressure for the points where a gas phase exists is shown in Figure 7. Maximal pressure is 5.2 MPa, obtained shortly before 10,000 years. Other teams participating in the benchmark obtained similar results, with the highest pressures oscillating between 5 and 5.5 MPa. The equivalent values for liquid pressure are shown in Figure 8.

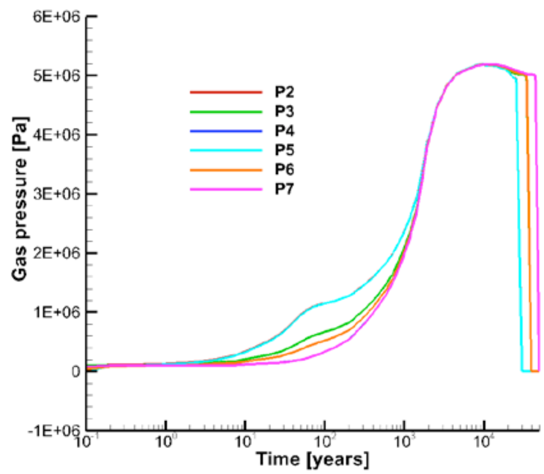

Figure 7. Values of the gas pressure at different points.

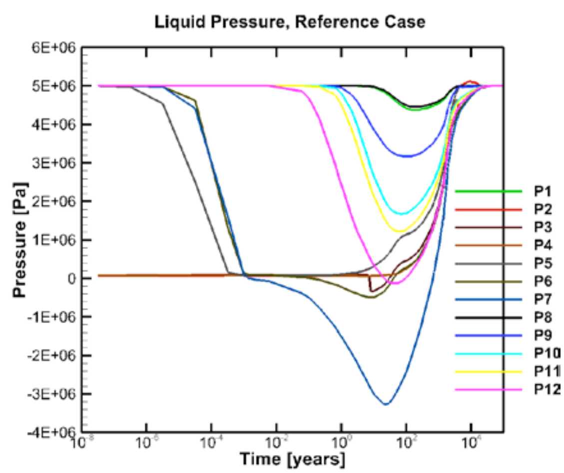

Figure 8. Values of the liquid pressure at different points.

Figure 9 shows values of the flux of gas and liquid through the drift and through the EDZ. A maximal flux of around 0.15 kg/a is obtained after 200 years. Afterwards, the flux decreases slowly up to the end of the gas generation period at 10,000 years. Comparing these values with the values of the liquid flux, we conclude that most of the hydrogen is being transported in a gas phase, with only a small part transported and dissolved in a liquid phase. Based on this figure we further conclude that most of the gas flux **migrates** first along the interface and then, when the peak of flux through the drift is reached, the flux through the EDZ starts increasing to reach a maximum at 10,000 years.

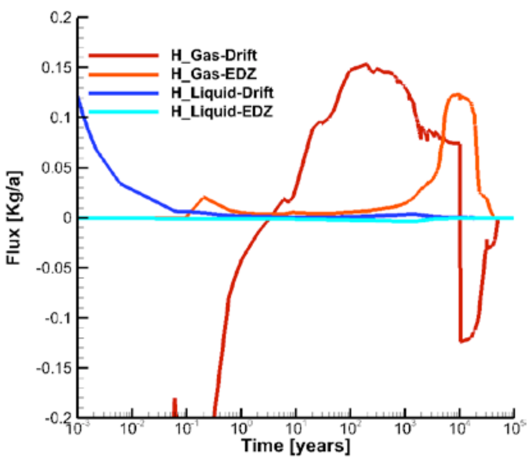

Figure 9. Flux of hydrogen in gas form and dissolved through the EDZ and through the drift for the reference case.

INFLUENCE OF THE MESH REFINEMENT

Figure 11 shows a detail of the grid with 2,500 nodes used for the reference case, generated with the program WinGridder (Pan 2001).

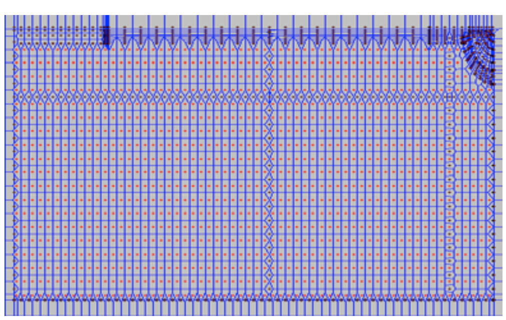

Figure 10. Mesh with 2500 nodes used for the calculations shown in this report.

The effect of mesh refinement was analyzed as prescribed in sensitivity analysis 6 (Table 3). Three different meshes were used, as shown in Table *4*; we concluded that the results of the calculations with the different meshes are similar. One difference, however, is that much more computation time is consumed than in the simulations, as shown in Table *4*. All the meshes considered have one layer of nodes in the interface.

Table 4. Different meshes used for sensitivity analysis 6.

	Computation time
Mesh 1: 2500 nodes	1-3 days
Mesh 2: 6300 nodes	2-7 days
Mesh 3: 1200 nodes	6-14 days

A detail of the mesh with 6200 nodes is shown in the next figure.

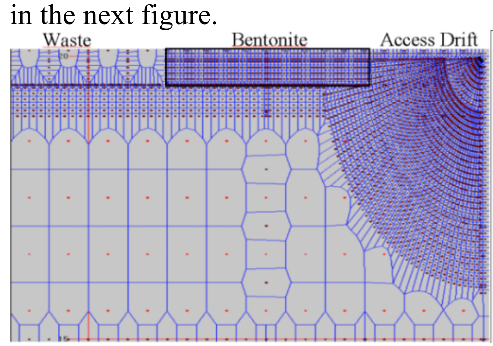

Figure 11. Detail of the nonconformal Voronoi mesh used to solve this exercise.

SOME RESULTS OF THE SENSITIVITY ANALYSES

In sensitivity analysis 1, only the intrinsic permeability of the EDZ for both drift and cell is changed to the same value as in the undisturbed rock. The resistance to the gas transport along the EDZ pathway is now higher; we expect (as shown in Figure 12) an increase in gas pressure close to the EDZ, compared to the reference scenario in Figure 7.

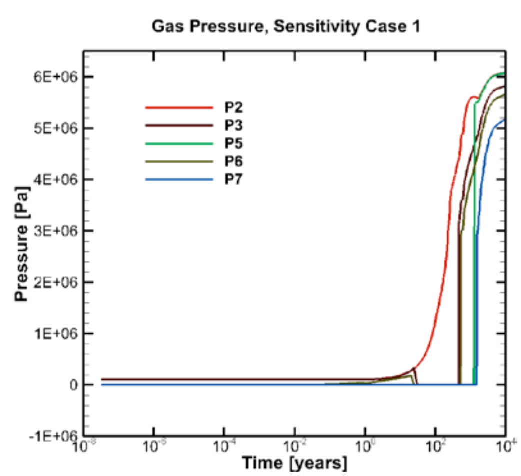

Figure 12. Values of the gas pressure at different points for sensitivity analysis 1.

As also expected, the liquid pressure decreases slower than in the reference case, and the minimal values of the pressure are higher than in the reference case—compare Figure 13 with Figure 8.

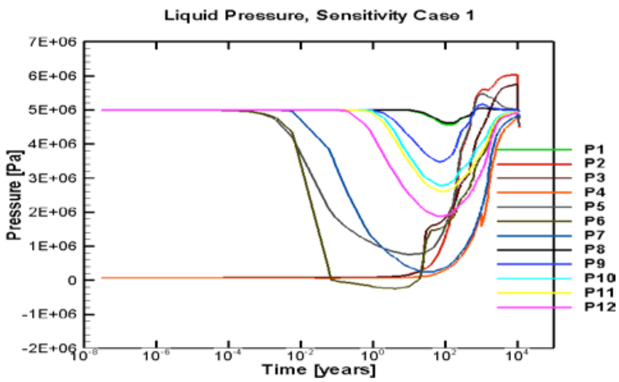

Figure 13. Values of the liquid pressure at different points for sensitivity analysis 1.

In sensitivity analysis 2 the permeability curve for EDZ water and gas, and of the undisturbed rock, follows a power law:

$$K_r^w = S_w^3 \qquad K_r^g = S_g^3 = (1 - S_w)^3 \qquad [7]$$

The influence of inserting expression (7) for the relative permeability can be seen when comparing Figure 14 with Figure 8. In fact, the minimal values of the water pressure are higher than in the reference case (see Figure 8). On the other hand, the values of the gas flux through the drift are the same as in the reference case. As the relative permeability function for the interface is not changed in this sensitivity analysis, this result confirms that the pathway through the interface is very important for gas transport.

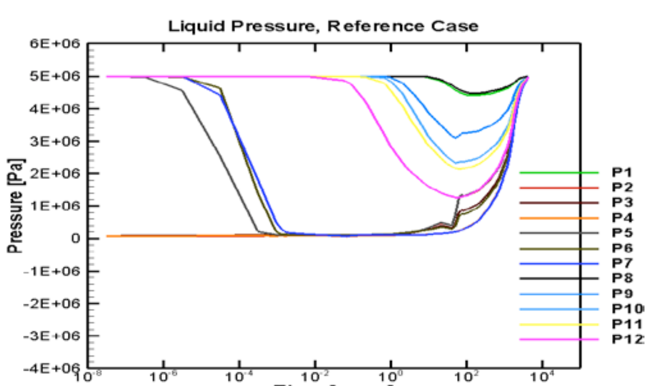

Figure 14. Values of the liquid pressure at different points for sensitivity analysis 2.

In sensitivity analysis 3 the diffusion coefficient of dissolved hydrogen under water-saturated conditions is incremented by a factor of 10 (Table 1 and Table 2) for all materials in the model.

In Figure 15, the gas flux for this sensitivity analysis is compared with the results from the reference scenario and from sensitivity analysis 1. In the case of sensitivity analysis 1, the gas flux through the drift increases mainly along the interface as the permeability of the EDZ increased. In the same figure, we can see that the increase of the diffusion coefficient of dissolved hydrogen has a significant impact on the total gas flow through the drift. For sensitivity analyses 2, 4a, 4b, 5a, 5b and 6 (see Table 3), the results of the flux through the drift are close to the ones of the reference case.

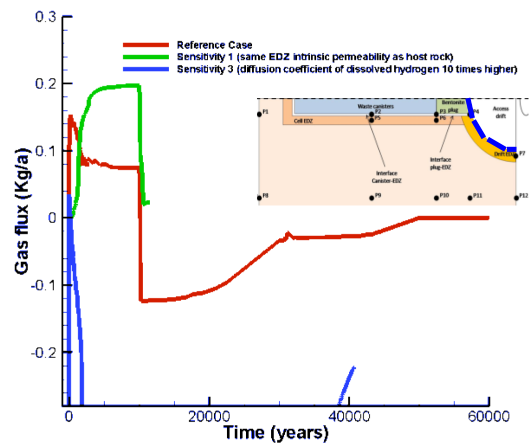

Figure 15. Comparison of gas flux through the drift for the reference case and sensitivity cases 1 and 3. The considered surface for the drift flux is indicated in the model.

In sensitivity analysis 4, the effect of a delay at the beginning of gas production of 1 year and of 2 years was simulated. These variations cause negligible differences in the results, as can be seen in Figure 16.

In sensitivity analysis 5, the permeability of the interface facing the canister was changed from $1.0{\times}10^{-12}$ m^2 to $1.0{\times}10^{-15}$ m^2 in sensitivity case 5a and to $1.0{\times}10^{-18}$ m^2, the same value as in the EDZ, in sensitivity case 5b. The results of this sensitivity analysis show that the gas keeps being transported along the same pathway— that is to say, the EDZ and the interface are main pathways around the drift.

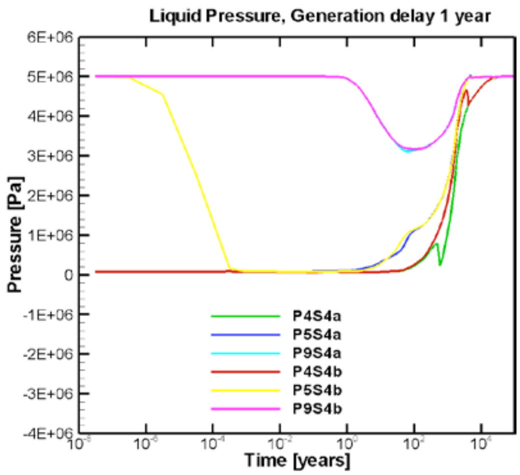

Figure 16. Values of the liquid pressure at different points for sensitivity analysis 4.

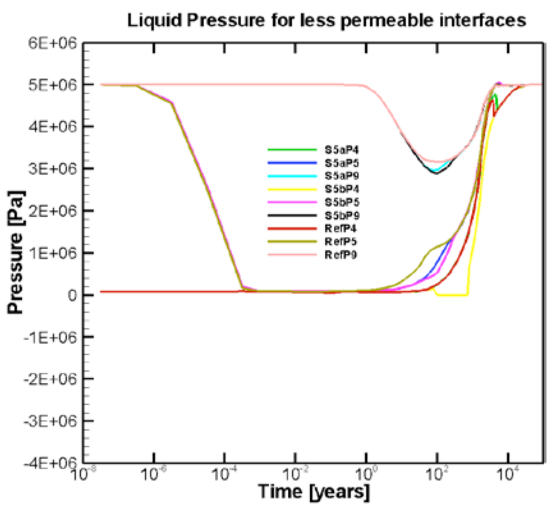

Figure 17. Values of the liquid pressure at different points for sensitivity analysis 5.

CONCLUSIONS

As result of this benchmark test, the following conclusions can be drawn:

- In order to represent the model and parameters as prescribed in the exercise, modifications of the codes TOUGH2/ TOUGH2-MP had to be made.
- The implementation of a interface in the model caused many numerical difficulties (convergence, increase in computation time).
- The interface and the EDZ represent the main pathway for migration of the hydrogen from the drift. The hydrogen is transported mainly in gas form and through the interface and EDZ.
- Implementing the expression for relative permeability as specified in the exercise caused many convergence problems; these problems disappeared using the original expression used in the TOUGH2/TOUGH2-MP code.
- Calculation time increases with the refinement of the mesh (Table 2), whereas the simulation results did not change significantly.
- The flux toward the drift increases with a low-permeable EDZ (sensitivity 1). Increasing the diffusion coefficient by a factor of 10 (sensitivity 3) decreases the flux toward the drift (Fig. 10, right).
- The results of the different teams are similar and within the same order of magnitude. Differences could be explained as resulting from the various approaches and simplifications to the model. Some differences were found in the values of the fluxes.

ACKNOWLEDGMENT

The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under Grant Agreement no230357, the FORGE project.

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